

VARIATIONAL FORMULATIONS FOR A HYDROGEN
NUCLEAR FUSION CHEMICAL REACTION INCLUDING
AN EULERIAN CONTEXT

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Abstract

This article develops variational formulations for a chemical reaction corresponding to a hydrogen nuclear fusion. The results are obtained through standard tools of calculus of variations and optimization theory in function spaces.

In such a chemical reaction, at an appropriate high temperature, a Deuterium ion reacts with a Tritium one resulting a Helium ion and an energetic neutron.

We highlight such a reaction result of an energetic neutron field has a great variety of practical applications, including the possibility of clean electric energy production.

Finally, we also emphasize in the last sections the results have been developed in an Eulerian context.

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1 Introduction

In this article we obtain variational formulations for modeling a hydrogen nuclear fusion in a high temperature process.

Recalling that a deuterium hydrogen atom is comprised by one proton, one neutron and one electron, a tritium hydrogen atom is comprised by one proton, two neutrons and one electron, a helium atom is comprised by two protons, two neutrons and two electrons, we consider a gas comprised by deuterium and an amount of tritium, which at a high temperature are ionized resulting in a plasma which chemically reacts resulting in a helium field and an energetic neutron one.

Such a chemical reaction may be summarized by the following equation



In terms of mass we shall represent this reaction as it follows:

$$1 = \alpha_D + \alpha_T = \alpha_{He} + \alpha_N,$$

that is, a unit mass fraction α_D of Deuterium reacts with a unit mass fraction α_T of tritium, resulting in a unit mass fraction α_{He} of Helium and a unit mass fraction α_N of neutrons.

We emphasize the results here presented have been obtained through standard tools of calculus of variations, basic constrained optimization and related Lagrange multipliers approach in infinite dimensional spaces.

Furthermore, as standard references in theoretical fluid mechanics we would cite [1, 2, 3, 4, 5, 6]. For related numerical methods we would mention [7, 8, 9]. Concerning similar models, we would cite [10, 11, 12, 13, 14].

Finally, details on the Sobolev and other function spaces involved may be found in [15].

2 The main variational formulation for a Lagrangian approach

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Denoting time by t we consider such a nuclear fusion process develops in Ω on a time interval $[0, t_f]$, so that $t \in [0, t_f]$.

We define the following density fields:

For the Deuterium proton,

$$\rho_D^p(x, y, z, t) = |\hat{\phi}_D^p(x, y, z, t)|^2 |\phi_D^A(y, z, t)|^2 |\phi_D(z, t)|^2 \frac{m_p}{m_D^A} \equiv |\phi_D^p(x, y, z, t)|^2,$$

Here, ρ_D^p stands for the density of a proton field in (x, y, z, t) , at an Deuterium atom with density at (y, z, t) and with a macroscopic Deuterium density in $(z, t) \in \Omega \times [0, t_f]$.

Similarly, for the Deuterium neutron density field, we define

$$\rho_D^N(x, y, z, t) = |\hat{\phi}_D^N(x, y, z, t)|^2 |\phi_D^A(y, z, t)|^2 |\phi_D(z, t)|^2 \frac{m_N}{m_D^A} \equiv |\phi_D^N(x, y, z, t)|^2.$$

For the Tritium proton field

$$\rho_T^p(x, y, z, t) = |\hat{\phi}_T^p(x, y, z, t)|^2 |\phi_T^A(y, z, t)|^2 |\phi_T(z, t)|^2 \frac{m_p}{m_T^A} \equiv |\phi_T^p(x, y, z, t)|^2.$$

and for the tritium neutron fields

$$\rho_T^{N1}(x, y, z, t) = |\hat{\phi}_T^{N1}(x, y, z, t)|^2 |\phi_T^A(y, z, t)|^2 |\phi_T(z, t)|^2 \frac{m_N}{m_T^A} \equiv |\phi_T^{N1}(x, y, z, t)|^2$$

and

$$\rho_T^{N2}(x, y, z, t) = |\hat{\phi}_T^{N2}(x, y, z, t)|^2 |\phi_T^A(y, z, t)|^2 |\phi_T(z, t)|^2 \frac{m_N}{m_T^A} \equiv |\phi_T^{N2}(x, y, z, t)|^2.$$

For the Helium protons, we define

$$\rho_{He}^{p1}(x, y, z, t) = |\hat{\phi}_{He}^{p1}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_p}{m_{He}^A} \equiv |\phi_{He}^{p1}(x, y, z, t)|^2$$

and

$$\rho_{He}^{p2}(x, y, z, t) = |\hat{\phi}_{He}^{p2}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_p}{m_{He}^A} \equiv |\phi_{He}^{p2}(x, y, z, t)|^2.$$

For the Helium neutron fields

$$\rho_{He}^{N1}(x, y, z, t) = |\hat{\phi}_{He}^{N1}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_N}{m_{He}^A} \equiv |\phi_{He}^{N1}(x, y, z, t)|^2$$

and

$$\rho_{He}^{N2}(x, y, z, t) = |\hat{\phi}_{He}^{N2}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_N}{m_{He}^A} \equiv |\phi_{He}^{N2}(x, y, z, t)|^2.$$

For the single neutron field

$$\rho_N(y, z, t) = |\hat{\phi}_N(y, z, t)|^2 |\phi_N^M(z, t)|^2 \equiv |\phi_N(y, z, t)|^2$$

where ϕ_N^M denotes the macroscopic neutron density field.

Finally, for the electronic field resulting from the ionization of Deuterium and Tritium atoms,

$$\rho_e = |\hat{\phi}_e(y, z, t)|^2 |\phi_e^M(z, t)|^2 \equiv |\phi_e(y, z, t)|^2$$

where again ϕ_e^M denotes the macroscopic electronic density field.

The corresponding position fields stand for:

For the Deuterium proton

$$\mathbf{r}_D^p(x, y, z, t) = \mathbf{r}_D(z, t) + \mathbf{r}_D^A(y, z, t) + \hat{\mathbf{r}}_D^p(x, y, z, t),$$

where $\mathbf{r}_D(z, t)$ is the macroscopic Deuterium position field in (z, t) , $\mathbf{r}_D^A(y, z, t)$ refers to the atom position field in (y, z, t) and $\hat{\mathbf{r}}_D^p(x, y, z, t)$ is the microscopic proton position field.

Similarly, for the Deuterium neutron position field we denote

$$\mathbf{r}_D^N(x, y, z, t) = \mathbf{r}_D(z, t) + \mathbf{r}_D^A(y, z, t) + \hat{\mathbf{r}}_D^N(x, y, z, t).$$

For the tritium proton

$$\mathbf{r}_T^p(x, y, z, t) = \mathbf{r}_T(z, t) + \mathbf{r}_T^A(y, z, t) + \hat{\mathbf{r}}_T^p(x, y, z, t),$$

and for the tritium neutron fields

$$\mathbf{r}_T^{N_1}(x, y, z, t) = \mathbf{r}_T(z, t) + \mathbf{r}_T^A(y, z, t) + \hat{\mathbf{r}}_T^{N_1}(x, y, z, t)$$

and

$$\mathbf{r}_T^{N_2}(x, y, z, t) = \mathbf{r}_T(z, t) + \mathbf{r}_T^A(y, z, t) + \hat{\mathbf{r}}_T^{N_2}(x, y, z, t).$$

For the Helium proton position fields, we denote

$$\mathbf{r}_{He}^{p_1}(x, y, z, t) = \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, z, t) + \hat{\mathbf{r}}_{He}^{p_1}(x, y, z, t)$$

and

$$\mathbf{r}_{He}^{p_2}(x, y, z, t) = \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, z, t) + \hat{\mathbf{r}}_{He}^{p_2}(x, y, z, t).$$

For the Helium neutron fields, we denote

$$\mathbf{r}_{He}^{N_1}(x, y, z, t) = \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, z, t) + \hat{\mathbf{r}}_{He}^{N_1}(x, y, z, t)$$

and

$$\mathbf{r}_{He}^{N_2}(x, y, z, t) = \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, z, t) + \hat{\mathbf{r}}_{He}^{N_2}(x, y, z, t).$$

For the neutron field

$$\mathbf{r}_N(y, z, t) = \mathbf{r}_N^M(z, t) + \hat{\mathbf{r}}_N(y, z, t)$$

Finally, for the electronic field resulting from ionization,

$$\mathbf{r}_e(y, z, t) = \mathbf{r}_e^M(z, t) + \hat{\mathbf{r}}_e(y, z, t)$$

The system is subject to the following constraints

$$\int_{\Omega} |\hat{\phi}_D^p(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_D^N(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_T^p(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_T^{N_1}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_T^{N_2}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{He}^{p_1}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{He}^{p_2}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{He}^{N_1}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{He}^{N_2}(x, y, z, t)|^2 dx = 1,$$

in $\Omega \times \Omega \times [0, t_f]$,

$$\int_{\Omega} |\hat{\phi}_N(y, z, t)|^2 dy = 1,$$

$$\int_{\Omega} |\hat{\phi}_e(y, z, t)|^2 dy = 1,$$

$$\int_{\Omega} |\phi_D^A(y, z, t)|^2 dy = 1,$$

$$\int_{\Omega} |\phi_T^A(y, z, t)|^2 dy = 1,$$

and

$$\int_{\Omega} |\hat{\phi}_{He}^A(y, z, t)|^2 dy = 1,$$

in $\Omega \times [0, t_f]$.

Defining

$$m_D(t) = \int_{\Omega} |\phi_D(z, t)|^2 dz,$$

$$m_T(t) = \int_{\Omega} |\phi_T(z, t)|^2 dz,$$

$$m_{H_e}(t) = \int_{\Omega} |\phi(z, t)_{H_e}|^2 dz,$$

$$m_N(t) = \int_{\Omega} |\phi_N^M(z, t)|^2 dz,$$

and

$$m_e(t) = \int_{\Omega} |\phi_e^M(z, t)|^2 dz,$$

and denoting

$$\rho_D(z, t) = |\phi_D(z, t)|^2,$$

$$\rho_T(z, t) = |\phi_T(z, t)|^2,$$

$$\rho_{H_e}(z, t) = |\phi_{H_e}(z, t)|^2,$$

$$\rho_N^M(z, t) = |\phi_N^M(z, t)|^2,$$

$$\rho_e^M(z, t) = |\phi_e^M(z, t)|^2,$$

and

$$\mathbf{v}_D = \frac{\partial \mathbf{r}_D(z, t)}{\partial t},$$

$$\mathbf{v}_T = \frac{\partial \mathbf{r}_T(z, t)}{\partial t},$$

$$\mathbf{v}_{H_e} = \frac{\partial \mathbf{r}_{H_e}(z, t)}{\partial t},$$

$$\mathbf{v}_N = \frac{\partial \mathbf{r}_N^M(z, t)}{\partial t},$$

and

$$\mathbf{v}_e = \frac{\partial \mathbf{r}_e^M(z, t)}{\partial t},$$

other constraints may be expressed by

$$\begin{aligned}
 m_D(t) &= (m_0)_D - \int_0^t \int_{\partial\Omega} \rho_D(z, \tau) \mathbf{v}_D(z, \tau) \cdot \mathbf{n} \, dS d\tau \\
 &\quad - \alpha_D [m_{He}(t) + m_N(t)] - \alpha_D \int_0^t \int_{\partial\Omega} \rho_{He}(z, \tau) \mathbf{v}_{He}(z, \tau) \cdot \mathbf{n} \, dS d\tau \\
 &\quad - \alpha_D \int_0^t \int_{\partial\Omega} \rho_N^M(z, \tau) \mathbf{v}_N(z, \tau) \cdot \mathbf{n} \, dS d\tau
 \end{aligned} \tag{1}$$

$$\begin{aligned}
 m_T(t) &= (m_0)_T - \int_0^t \int_{\partial\Omega} \rho_T(z, \tau) \mathbf{v}_T(z, \tau) \cdot \mathbf{n} \, dS d\tau \\
 &\quad - \alpha_T [m_{He}(t) + m_N(t)] - \alpha_T \int_0^t \int_{\partial\Omega} \rho_{He}(z, \tau) \mathbf{v}_{He}(z, \tau) \cdot \mathbf{n} \, dS d\tau \\
 &\quad - \alpha_T \int_0^t \int_{\partial\Omega} \rho_N^M(z, \tau) \mathbf{v}_N(z, \tau) \cdot \mathbf{n} \, dS d\tau
 \end{aligned} \tag{2}$$

$$\begin{aligned}
 &\alpha_N \left(m_{He}(t) + \int_0^t \int_{\partial\Omega} \rho_{He}(z, \tau) \mathbf{v}_{He}(z, \tau) \cdot \mathbf{n} \, dS d\tau \right) \\
 &= \alpha_{He} \left(m_N(t) + \int_0^t \int_{\partial\Omega} \rho_N^M(z, \tau) \mathbf{v}_N(z, \tau) \cdot \mathbf{n} \, dS d\tau \right)
 \end{aligned} \tag{3}$$

$$m_e(t) = (m_0)_e - \int_0^t \int_{\partial\Omega} \rho_e^M(z, \tau) \mathbf{v}_e(z, \tau) \cdot \mathbf{n} \, dS d\tau, \tag{4}$$

where $\mathbf{n}$ denotes the outward normal field to $\partial\Omega = S$.

At this point, we define the kinetics energy functional E_C by

$$\begin{aligned}
 E_c = & \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^p \frac{\partial \mathbf{r}_D^p}{\partial t} \cdot \frac{\partial \mathbf{r}_D^p}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^N \frac{\partial \mathbf{r}_D^N}{\partial t} \cdot \frac{\partial \mathbf{r}_D^N}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^p \frac{\partial \mathbf{r}_T^p}{\partial t} \cdot \frac{\partial \mathbf{r}_T^p}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_1} \frac{\partial \mathbf{r}_T^{N_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_T^{N_1}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_2} \frac{\partial \mathbf{r}_T^{N_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_T^{N_2}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{p_1} \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{p_2} \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_1} \frac{\partial \mathbf{r}_{He}^{N_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{N_1}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_2} \frac{\partial \mathbf{r}_{He}^{N_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{N_2}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_N \frac{\partial \mathbf{r}_N}{\partial t} \cdot \frac{\partial \mathbf{r}_N}{\partial t} dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_e \frac{\partial \mathbf{r}_e}{\partial t} \cdot \frac{\partial \mathbf{r}_e}{\partial t} dy dz dt,
 \end{aligned} \tag{5}$$

Here we define the functional E_q where

$$\begin{aligned}
 E_q = & \frac{\gamma_D^p}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_D^p - iw_D^p \mathbf{A}(z, t) \phi_D^p|^2 dx dy dz dt \\
 & + \frac{\gamma_D^N}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_D^N - iw_D^N \mathbf{A}(z, t) \phi_D^N|^2 dx dy dz dt \\
 & + \frac{\gamma_T^p}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_T^p - iw_T^p \mathbf{A}(z, t) \phi_T^p|^2 dx dy dz dt \\
 & + \frac{\gamma_T^{N_1}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_T^{N_1} - iw_T^{N_1} \mathbf{A}(z, t) \phi_T^{N_1}|^2 dx dy dz dt \\
 & + \frac{\gamma_T^{N_2}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_T^{N_2} - iw_T^{N_2} \mathbf{A}(z, t) \phi_T^{N_2}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{p_1}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{p_1} - iw_{H_e}^{p_1} \mathbf{A}(z, t) \phi_{H_e}^{p_1}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{p_2}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{p_2} - iw_{H_e}^{p_2} \mathbf{A}(z, t) \phi_{H_e}^{p_2}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{N_1}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{N_1} - iw_{H_e}^{N_1} \mathbf{A}(z, t) \phi_{H_e}^{N_1}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{N_2}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{N_2} - iw_{H_e}^{N_2} \mathbf{A}(z, t) \phi_{H_e}^{N_2}|^2 dx dy dz dt \\
 & + \frac{\gamma_N}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_N - iw_N \mathbf{A}(z, t) \phi_N|^2 dy dz dt \\
 & + \frac{\gamma_e}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_e - iw_e \mathbf{A}(z, t) \phi_e|^2 dy dz dt \\
 & + \frac{\gamma_D^A}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_D^A - iw_D^A \mathbf{A}(z, t) \phi_D^A|^2 dy dz dt \\
 & + \frac{\gamma_T^A}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_T^A - iw_T^A \mathbf{A}(z, t) \phi_T^A|^2 dy dz dt \\
 & + \frac{\gamma_{H_e}^A}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_{H_e}^A - iw_{H_e}^A \mathbf{A}(z, t) \phi_{H_e}^A|^2 dy dz dt \\
 & + \frac{\gamma_D}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_D - iw_D \mathbf{A}(z, t) \phi_D|^2 dz dt \\
 & + \frac{\gamma_T}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_T - iw_T \mathbf{A}(z, t) \phi_T|^2 dz dt \\
 & + \frac{\gamma_{H_e}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_{H_e} - iw_{H_e} \mathbf{A}(z, t) \phi_{H_e}|^2 dz dt \\
 & + \frac{\gamma_N^M}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_N^M - iw_N^M \mathbf{A}(z, t) \phi_N^M|^2 dz dt \\
 & + \frac{\gamma_e^M}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_e^M - iw_N^M \mathbf{A}(z, t) \phi_e^M|^2 dz dt. \tag{6}
 \end{aligned}$$

We define also,

$$\begin{aligned}
 E_{q_1} = & \frac{\gamma_D^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_D}{\partial t} \cdot \frac{\partial \phi_D}{\partial t} dz dt \\
 & + \frac{\gamma_T^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_T}{\partial t} \cdot \frac{\partial \phi_T}{\partial t} dz dt \\
 & + \frac{\gamma_{He}^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_{He}}{\partial t} \cdot \frac{\partial \phi_{He}}{\partial t} dz dt \\
 & + \frac{\gamma_N^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_N^M}{\partial t} \cdot \frac{\partial \phi_N^M}{\partial t} dx dt \\
 & + \frac{\gamma_e^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_e^M}{\partial t} \cdot \frac{\partial \phi_e^M}{\partial t} dz dt.
 \end{aligned} \tag{7}$$

For the interaction energy functional we consider only a simplified self interaction part, denoted by E_{int} , where

$$\begin{aligned}
 E_{int} = & \frac{\alpha_D}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_D|^4 dx dy dz dt \\
 & + \frac{\alpha_T}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_T|^4 dx dy dz dt \\
 & + \frac{\alpha_{He}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}|^4 dx dy dz dt \\
 & + \frac{\alpha_N}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\phi_N|^4 dy dz dt \\
 & + \frac{\alpha_e}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\phi_e|^4 dy dz dt.
 \end{aligned} \tag{8}$$

Furthermore, concerning the scalar temperature field, we define

$$\begin{aligned}
 (C_v)_{D\rho_D}(z, t) T_D(z, t) = & \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^p|^2 \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \right) dx dy \\
 & + \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^N|^2 \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \right) dx dy
 \end{aligned} \tag{9}$$

$$\begin{aligned}
 (C_v)_{T\rho_T}(z, t) T_T(z, t) = & \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^p|^2 \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \right) dx dy \\
 & + \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \right) dx dy \\
 & + \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \right) dx dy
 \end{aligned} \tag{10}$$

$$\begin{aligned}
(C_v)_{H_e} \rho_{H_e}(z, t) T_{H_e}(z, t) &= \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{p_1}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_1}}{\partial t} \right) dx dy \\
&+ \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{p_2}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_2}}{\partial t} \right) dx dy \\
&+ \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_1}}{\partial t} \right) dx dy \\
&+ \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_2}}{\partial t} \right) dx dy \quad (11)
\end{aligned}$$

$$(C_v)_N \rho_N^M(z, t) T_N(z, t) = \int_{\Omega} \left(\frac{1}{2} |\phi_N|^2 \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \right) dy \quad (12)$$

$$(C_v)_e \rho_e^M(z, t) T_e = \int_{\Omega} \left(\frac{1}{2} |\phi_e|^2 \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \right) dy \quad (13)$$

Moreover, we define

$$T(z, t) = T_D + T_T + T_{H_e} + T_N + T_e$$

and similarly as indicated in [16] for a non-viscous fluid, we also assume the following constraint

$$\begin{aligned}
&|\phi_D|^2 (C_v)_D \frac{\partial T_D}{\partial t} + |\phi_T|^2 (C_v)_T \frac{\partial T_T}{\partial t} \\
&+ |\phi_{H_e}|^2 (C_v)_{H_e} \frac{\partial T_{H_e}}{\partial t} + |\phi_N|^2 (C_v)_N \frac{\partial T_N}{\partial t} + |\phi_e|^2 (C_v)_e \frac{\partial T_e}{\partial t} \\
&- K_D \nabla^2 T_D - K_T \nabla^2 T_T - K_{H_e} \nabla^2 T_{H_e} - K_N \nabla^2 T_N - K_e \nabla^2 T_e \\
&+ P_D \operatorname{div} \mathbf{v}_D + P_T \operatorname{div} \mathbf{v}_T + P_{H_e} \operatorname{div} \mathbf{v}_{H_e} \\
&+ P_N \operatorname{div} \mathbf{v}_N + P_e \operatorname{div} \mathbf{v}_e - \frac{\partial Q}{\partial t} = 0, \text{ in } \Omega \times [0, t_f], \quad (14)
\end{aligned}$$

where Q is a heat function and

$$\begin{aligned}
P_D &= \frac{d(\hat{P} \rho_D)}{dt}, \\
P_T &= \frac{d(\hat{P} \rho_T)}{dt}, \\
P_{H_e} &= \frac{d(\hat{P} \rho_{H_e})}{dt},
\end{aligned}$$

$$P_N = \frac{d(\hat{P}\rho_N)}{dt},$$

and

$$P_e = \frac{d(\hat{P}\rho_e)}{dt}.$$

Finally, we assume the following mass conservation equation as a constraint

$$\begin{aligned} & \frac{d\rho}{dt} + \rho_D \operatorname{div}(\mathbf{v}_D) + \rho_T \operatorname{div}(\mathbf{v}_T) \\ & + \rho_{H_e} \operatorname{div}(\mathbf{v}_{H_e}) + \rho_N \operatorname{div}(\mathbf{v}_N) \\ & + \rho_e \operatorname{div}(\mathbf{v}_e) = 0, \text{ in } \Omega \times [0, t_f], \end{aligned} \quad (15)$$

where we have denoted for not relabeled functions

$$\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e$$

and

$$\begin{aligned} \rho_D &= \rho_D(\mathbf{r}_D(z, t), t), \\ \rho_T &= \rho_T(\mathbf{r}_T(z, t), t), \\ \rho_{H_e} &= \rho_{H_e}(\mathbf{r}_{H_e}(z, t), t), \\ \rho_N &= \rho_N(\mathbf{r}_N^M(z, t), t), \end{aligned}$$

and

$$\rho_e = \rho_e(\mathbf{r}_e^M(z, t), t).$$

In order to model such a chemical reaction, we define the following functional J , which corresponds to a variational formulation for the model in question, where

$$\begin{aligned} J &= E_C + E_q + E_{q_1} + E_{int} \\ &- \int_0^{t_f} \int_{\Omega} \hat{P} \left(\frac{d\rho}{dt} + \rho_D \operatorname{div}(\mathbf{v}_D) + \rho_T \operatorname{div}(\mathbf{v}_T) \right. \\ &+ \rho_{H_e} \operatorname{div}(\mathbf{v}_{H_e}) + \rho_N \operatorname{div}(\mathbf{v}_N) \\ &+ \rho_e \operatorname{div}(\mathbf{v}_e) \Big) dz dt \\ &+ J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4} + J_{Aux_5} + J_{Aux_6}, \end{aligned} \quad (16)$$

where

$$\begin{aligned}
J_{Aux_1} = & \int_0^{t_f} \int_{\Omega} \lambda_D \left((C_v)_D \rho_D(z, t) T_D(z, t) - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^p|^2 \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^N|^2 \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \right) dx dy \right) dz dt \\
& - \int_0^{t_f} \int_{\Omega} \lambda_T \left((C_v)_T \rho_T(z, t) T_T(z, t) - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^p|^2 \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \right) dx dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_{He} \left((C_v)_{He} \rho_{He}(z, t) T_{He}(z, t) - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{He}^{p_1}|^2 \frac{\partial \hat{\mathbf{r}}_{He}^{p_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{p_1}}{\partial t} \right) dx dy \right. \\
& - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{He}^{p_2}|^2 \frac{\partial \hat{\mathbf{r}}_{He}^{p_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{p_2}}{\partial t} \right) dx dy \\
& - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{He}^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_{He}^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{N_1}}{\partial t} \right) dx dy \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{He}^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_{He}^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{N_2}}{\partial t} \right) dx dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_N \left((C_v)_N \rho_N^M(z, t) T_N(z, t) - \int_{\Omega} \left(\frac{1}{2} |\phi_N|^2 \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \right) dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_e \left((C_v)_e \rho_e^M(z, t) T_e - \int_{\Omega} \left(\frac{1}{2} |\phi_e|^2 \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \right) dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_1 \left(|\phi_D|^2 (C_v)_D \frac{\partial T_D}{\partial t} + |\phi_T|^2 (C_v)_T \frac{\partial T_T}{\partial t} \right. \\
& + |\phi_{He}|^2 (C_v)_{He} \frac{\partial T_{He}}{\partial t} + |\phi_N|^2 (C_v)_N \frac{\partial T_N}{\partial t} + |\phi_e|^2 (C_v)_e \frac{\partial T_e}{\partial t} \\
& - K_D \nabla^2 T_D - K_T \nabla^2 T_T - K_{He} \nabla^2 T_{He} - K_N \nabla^2 T_N - K_e \nabla^2 T_e \\
& + P_D \operatorname{div} \mathbf{v}_D + P_T \operatorname{div} \mathbf{v}_T + P_{He} \operatorname{div} \mathbf{v}_{He} \\
& \left. + P_N \operatorname{div} \mathbf{v}_N + P_e \operatorname{div} \mathbf{v}_e - \frac{\partial Q}{\partial t} \right) dz dt, \tag{17}
\end{aligned}$$

Moreover,

$$\begin{aligned}
 J_{Aux_2} = & \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_D^p(y, z, t) \left(\int_{\Omega} |\hat{\phi}_D^p(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_D^p(y, z, t) \left(\int_{\Omega} |\hat{\phi}_D^N(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_T^p(y, z, t) \left(\int_{\Omega} |\hat{\phi}_T^p(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_T^{N_1}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_T^{N_1}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_T^{N_2}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_T^{N_2}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{p_1}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{p_1}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{p_2}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{p_2}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{N_1}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{N_1}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{N_2}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{N_2}(x, y, z, t)|^2 dx - 1 \right) dydzdt \quad (18)
 \end{aligned}$$

$$\begin{aligned}
 J_{Aux_3} = & \int_0^{t_f} \int_{\Omega} E_N(z, t) \left(\int_{\Omega} \int_{\Omega} |\hat{\phi}_N(y, z, t)|^2 dy - 1 \right) dzdt, \\
 & + \int_0^{t_f} \int_{\Omega} E_e(z, t) \left(\int_{\Omega} |\hat{\phi}_e(y, z, t)|^2 dy - 1 \right) dzdt, \\
 & + \int_0^{t_f} \int_{\Omega} E_D^A(z, t) \left(\int_{\Omega} |\phi_D^A(y, z, t)|^2 dy - 1 \right) dzdt \\
 & + \int_0^{t_f} \int_{\Omega} E_T^A(z, t) \left(\int_{\Omega} |\phi_T^A(y, z, t)|^2 dy - 1 \right) dzdt \\
 & + \int_0^{t_f} \int_{\Omega} E_{H_e}^A(z, t) \left(\int_{\Omega} |\phi_{H_e}^A(y, z, t)|^2 dy - 1 \right) dzdt \quad (19)
 \end{aligned}$$

and denoting

$$\begin{aligned}
 & J_{Aux_4} \\
 = & \int_0^{t_f} \mu_D(t) \left(m_D(t) - (m_0)_D + \int_0^t \int_{\partial\Omega} \rho_D(z, \tau) \mathbf{v}_D(z, \tau) \cdot \mathbf{n} \, dS d\tau \right. \\
 & + \alpha_D [m_{He}(t) + m_N(t)] - \alpha_D \int_0^t \int_{\partial\Omega} \rho_{He}(z, \tau) \mathbf{v}_{He}(z, \tau) \cdot \mathbf{n} \, dS d\tau \\
 & \left. + \alpha_D \int_0^t \int_{\partial\Omega} \rho_N(z, \tau) \mathbf{v}_N(z, \tau) \cdot \mathbf{n} \, dS d\tau \right) dt \\
 & + \int_0^{t_f} \mu_T(t) \left(m_T(t) - (m_0)_T + \int_0^t \int_{\partial\Omega} \rho_T(z, \tau) \mathbf{v}_T(z, \tau) \cdot \mathbf{n} \, dS d\tau \right. \\
 & + \alpha_T [m_{He}(t) + m_N(t)] + \alpha_T \int_0^t \int_{\partial\Omega} \rho_{He}(z, \tau) \mathbf{v}_{He}(z, \tau) \cdot \mathbf{n} \, dS d\tau \\
 & \left. + \alpha_T \int_0^t \int_{\partial\Omega} \rho_N(z, \tau) \mathbf{v}_N(z, \tau) \cdot \mathbf{n} \, dS d\tau \right) dt \\
 & + \int_0^{t_f} \mu_3(t) \left(\alpha_N \left(m_{He}(t) + \int_0^t \int_{\partial\Omega} \rho_{He}(z, \tau) \mathbf{v}_{He}(z, \tau) \cdot \mathbf{n} \, dS d\tau \right) \right. \\
 & \left. - \alpha_{He} \left(m_N(t) + \int_0^t \int_{\partial\Omega} \rho_N(z, \tau) \mathbf{v}_N(z, \tau) \cdot \mathbf{n} \, dS d\tau \right) \right) dt \\
 & + \int_0^{t_f} \mu_4(t) \left(m_e(t) - (m_0)_e + \int_0^t \int_{\partial\Omega} \rho_e^M(z, \tau) \mathbf{v}_e(z, \tau) \cdot \mathbf{n} \, dS d\tau \right) dt \quad (20)
 \end{aligned}$$

Furthermore,

$$\begin{aligned}
 & J_{Aux5} \\
 = & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} V(\mathbf{r}_D^p, \mathbf{r}_T^p, \mathbf{r}_{He}^{p_1}, \mathbf{r}_{He}^{p_2}, \mathbf{r}_e) \\
 & \times (|\phi_D^p|^2 + |\phi_T^p|^2 + |\phi_{He}^{p_1}|^2 + |\phi_{He}^{p_2}|^2 + |\phi_e|^2) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_D^p|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_D^p}{\partial t} \cdot (\mathbf{r}_D^p(z, \varepsilon t) - (\mathbf{r}_0)_D^p) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_T^p|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_T^p}{\partial t} \cdot (\mathbf{r}_T^p(z, \varepsilon t) - (\mathbf{r}_0)_T^p) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_1}|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} \cdot (\mathbf{r}_{He}^{p_1}(z, \varepsilon t) - (\mathbf{r}_0)_{He}^{p_1}) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_2}|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} \cdot (\mathbf{r}_{He}^{p_2}(z, \varepsilon t) - (\mathbf{r}_0)_{He}^{p_2}) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_e|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_e}{\partial t} \cdot (\mathbf{r}_e(z, \varepsilon t) - (\mathbf{r}_0)_e) dx dy dz dt \\
 & + \frac{1}{8\pi} \int_0^{t_f} \int_{\Omega} |\text{curl } \mathbf{A}(z, t) - \mathbf{B}_0(z, t)|^2 dz dt \\
 & + \frac{1}{8\pi} \int_0^{t_f} \int_{\Omega} \left| \int_{\Omega} \int_{\Omega} \nabla_z V(\mathbf{r}_D^p, \mathbf{r}_T^p, \mathbf{r}_{He}^{p_1}, \mathbf{r}_{He}^{p_2}, \mathbf{r}_e) dx dy + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right|^2 dz dt, \quad (21)
 \end{aligned}$$

where

$$\mathbf{B}(z, t) = \text{curl } \mathbf{A}(z, t) - \mathbf{B}_0(z, t)$$

is the total magnetic field,

$$\mathbf{A} = (A_1, A_2, A_3) \in W^{1,2}(\Omega \times [0, t_f]; \mathbb{R}^3)$$

denotes the magnetic potential and

$$\mathbf{E} = - \int_{\Omega} \int_{\Omega} \nabla_z V(\mathbf{r}_D^p, \mathbf{r}_T^p, \mathbf{r}_{He}^{p_1}, \mathbf{r}_{He}^{p_2}, \mathbf{r}_e) dx dy - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t},$$

denotes the electric field.

Finally,

$$\begin{aligned}
 J_{Aux_6} = & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_D^p|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_D^p}{\partial t} dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_T^p|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_T^p}{\partial t} dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_1}|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_2}|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} dx dy dz dt \\
 & -K_2 \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\phi_e|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_e}{\partial t} dy dz dt. \tag{22}
 \end{aligned}$$

Remark 2.1. About the domain of the functional J , we generically define it as sets of smooth C^2 functions, specifying only the following boundary and initial conditions

$$\mathbf{r} = (\mathbf{r}_D, \mathbf{r}_T, \mathbf{r}_{He}, \mathbf{r}_N^M, \mathbf{r}_e^M) = \mathbf{0}, \text{ on } \partial\Omega \times [0, t_f],$$

$$\mathbf{r}|_{t=0} = z, \text{ in } \Omega,$$

$$\mathbf{v} = (\mathbf{v}_D, \mathbf{v}_T, \mathbf{v}_{He}, \mathbf{v}_N^M, \mathbf{v}_e^M) = \mathbf{0}, \text{ on } \partial\Omega \times [0, t_f],$$

$$\mathbf{v}|_{t=0} = \mathbf{v}_0 \text{ in } \Omega,$$

$$T = T_0(z, t) \text{ on } \partial\Omega \times [0, t_f]$$

$$T|_{t=0} = T_1(z), \text{ in } \Omega$$

and

$$\rho|_{t=0} = (\rho_D, \rho_T, \rho_{He}, \rho_N, \rho_e)|_{t=0} = ((\rho_D)_0, (\rho_T)_0, 0, 0, (\rho_e)_0) \text{ in } \Omega.$$

Remark 2.2. Concerning the variation of J in $\mathbf{r}$, we consider variations in the context

$$(\mathbf{r} + h\varphi) \text{ and } (\mathbf{r}(\cdot, \varepsilon t) + h\varphi),$$

that is, the same variable variation φ and real constant h for both $\mathbf{r}$ and $\mathbf{r}(\cdot, \varepsilon t)$ for obtaining an approximate Euler-Lagrange equation. Finally, letting $\varepsilon \rightarrow 0$ we obtain the correct Euler-Lagrange equation.

Remark 2.3. With the boundary conditions we have set, surface integrals I_n similar as that below indicated equal zero, that is,

$$I_n = \int_0^t \int_{\partial\Omega} \rho_D(z, \tau) \mathbf{v}_D(z, \tau) \cdot \mathbf{n} dS d\tau = 0.$$

Anyway, we keep such more general expressions in the main functionals considering that, in the next sections, we address a more general approach with a concerning control volume and fields in an Eulerian context.

3 The main variational formulation for an Eulerian approach

Let $\Omega \subset \mathbb{R}^3$ be an open, bounded and connected set with a regular (Lipschitzian) boundary denoted by $\partial\Omega$.

Denoting time by t we consider such a nuclear fusion process develops in Ω on a time interval $[0, t_f]$, so that $t \in [0, t_f]$.

We define the following density fields:

For the Deuterium proton,

$$\rho_D^p(x, y, z, t) = |\hat{\phi}_D^p(x, y, z, t)|^2 |\phi_D^A(y, z, t)|^2 |\phi_D(z, t)|^2 \frac{m_p}{m_D^A} \equiv |\phi_D^p(x, y, z, t)|^2,$$

Here, ρ_D^p stands for the density of a proton field in (x, y, z, t) , at an Deuterium atom with density at (y, z, t) and with a macroscopic Deuterium density in $(z, t) \in \Omega \times [0, t_f]$.

Similarly, for the Deuterium neutron density field, we define

$$\rho_D^N(x, y, z, t) = |\hat{\phi}_D^N(x, y, z, t)|^2 |\phi_D^A(y, z, t)|^2 |\phi_D(z, t)|^2 \frac{m_N}{m_D^A} \equiv |\phi_D^N(x, y, z, t)|^2.$$

For the Tritium proton field

$$\rho_T^p(x, y, z, t) = |\hat{\phi}_T^p(x, y, z, t)|^2 |\phi_T^A(y, z, t)|^2 |\phi_T(z, t)|^2 \frac{m_p}{m_T^A} \equiv |\phi_T^p(x, y, z, t)|^2.$$

and for the tritium neutron fields

$$\rho_T^{N1}(x, y, z, t) = |\hat{\phi}_T^{N1}(x, y, z, t)|^2 |\phi_T^A(y, z, t)|^2 |\phi_T(z, t)|^2 \frac{m_N}{m_T^A} \equiv |\phi_T^{N1}(x, y, z, t)|^2$$

and

$$\rho_T^{N2}(x, y, z, t) = |\hat{\phi}_T^{N2}(x, y, z, t)|^2 |\phi_T^A(y, z, t)|^2 |\phi_T(z, t)|^2 \frac{m_N}{m_T^A} \equiv |\phi_T^{N2}(x, y, z, t)|^2.$$

For the Helium protons, we define

$$\rho_{He}^{p1}(x, y, z, t) = |\hat{\phi}_{He}^{p1}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_p}{m_{He}^A} \equiv |\phi_{He}^{p1}(x, y, z, t)|^2$$

and

$$\rho_{He}^{p2}(x, y, z, t) = |\hat{\phi}_{He}^{p2}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_p}{m_{He}^A} \equiv |\phi_{He}^{p2}(x, y, z, t)|^2.$$

For the Helium neutron fields

$$\rho_{He}^{N1}(x, y, z, t) = |\hat{\phi}_{He}^{N1}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_N}{m_{He}^A} \equiv |\phi_{He}^{N1}(x, y, z, t)|^2$$

and

$$\rho_{He}^{N2}(x, y, z, t) = |\hat{\phi}_{He}^{N2}(x, y, z, t)|^2 |\phi_{He}^A(y, z, t)|^2 |\phi_{He}(z, t)|^2 \frac{m_N}{m_{He}^A} \equiv |\phi_{He}^{N2}(x, y, z, t)|^2.$$

For the single neutron field

$$\rho_N(y, z, t) = |\hat{\phi}_N(y, z, t)|^2 |\phi_N^M(z, t)|^2 \equiv |\phi_N(y, z, t)|^2$$

where ϕ_N^M denotes the macroscopic neutron density field.

Finally, for the electronic field resulting from the ionization of Deuterium and Tritium atoms,

$$\rho_e = |\hat{\phi}_e(y, z, t)|^2 |\phi_e^M(z, t)|^2 \equiv |\phi_e(y, z, t)|^2$$

where again ϕ_e^M denotes the macroscopic electronic density field.

The corresponding position fields stand for:

For the Deuterium proton

$$\begin{aligned} \mathbf{r}_D^p(x, y, z, t) &= \mathbf{r}_D(z, t) + \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_D^p(x, \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t), \mathbf{r}_D(z, t), t) \\ &= \mathbf{r}_D(z, t) + \hat{\mathbf{r}}_D^p(x, y, \mathbf{r}_D(z, t), t), \end{aligned} \quad (23)$$

where

$$\tilde{\mathbf{r}}_D^p(x, y, \mathbf{r}_D(z, t), t) = \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t) + \tilde{\mathbf{r}}_D^p(x, \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t), \mathbf{r}_D(z, t), t).$$

Here $\mathbf{r}_D(z, t)$ is the macroscopic Deuterium position field in (z, t) ,

$$\mathbf{r}_D^A(y, \mathbf{r}(z, t), t)$$

refers to the atom position field in (y, z, t) and

$$\tilde{\mathbf{r}}_D^p(x, \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t), \mathbf{r}_D(z, t), t)$$

is the microscopic proton position field.

Similarly, for the Deuterium neutron position field we denote

$$\begin{aligned}\mathbf{r}_D^N(x, y, z, t) &= \mathbf{r}_D(z, t) + \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_D^N(x, \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t), \mathbf{r}_D(z, t), t) \\ &= \mathbf{r}_D(z, t) + \hat{\mathbf{r}}_D^N(x, y, \mathbf{r}_D(z, t), t),\end{aligned}\tag{24}$$

where

$$\hat{\mathbf{r}}_D^N(x, y, \mathbf{r}_D(z, t), t) = \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t) + \tilde{\mathbf{r}}_D^N(x, \mathbf{r}_D^A(y, \mathbf{r}_D(z, t), t), \mathbf{r}_D(z, t), t).$$

For the tritium proton

$$\begin{aligned}\mathbf{r}_T^p(x, y, z, t) &= \mathbf{r}_T(z, t) + \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_T^p(x, \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t), \mathbf{r}_T(z, t), t) \\ &= \mathbf{r}_T(z, t) + \hat{\mathbf{r}}_T^p(x, y, \mathbf{r}_T(z, t), t),\end{aligned}\tag{25}$$

where

$$\hat{\mathbf{r}}_T^p(x, y, \mathbf{r}_T(z, t), t) = \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t) + \tilde{\mathbf{r}}_T^p(x, \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t), \mathbf{r}_T(z, t), t).$$

and for the tritium neutron fields

$$\begin{aligned}\mathbf{r}_T^{N1}(x, y, z, t) &= \mathbf{r}_T(z, t) + \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_T^{N1}(x, \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t), \mathbf{r}_T(z, t), t) \\ &= \mathbf{r}_T(z, t) + \hat{\mathbf{r}}_T^{N1}(x, y, \mathbf{r}_T(z, t), t),\end{aligned}\tag{26}$$

where

$$\hat{\mathbf{r}}_T^{N1}(x, y, \mathbf{r}_T(z, t), t) = \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t) + \tilde{\mathbf{r}}_T^{N1}(x, \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t), \mathbf{r}_T(z, t), t).$$

and

$$\begin{aligned}\mathbf{r}_T^{N2}(x, y, z, t) &= \mathbf{r}_T(z, t) + \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_T^{N2}(x, \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t), \mathbf{r}_T(z, t), t) \\ &= \mathbf{r}_T(z, t) + \hat{\mathbf{r}}_T^{N2}(x, y, \mathbf{r}_T(z, t), t),\end{aligned}\tag{27}$$

where

$$\hat{\mathbf{r}}_T^{N2}(x, y, \mathbf{r}_T(z, t), t) = \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t) + \tilde{\mathbf{r}}_T^{N2}(x, \mathbf{r}_T^A(y, \mathbf{r}_T(z, t), t), \mathbf{r}_T(z, t), t).$$

For the Helium proton position fields, we denote

$$\begin{aligned}\mathbf{r}_{He}^{p1}(x, y, z, t) &= \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_{He}^{p1}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t) \\ &= \mathbf{r}_{He}(z, t) + \hat{\mathbf{r}}_{He}^{p1}(x, y, \mathbf{r}_{He}(z, t), t),\end{aligned}\tag{28}$$

where

$$\hat{\mathbf{r}}_{He}^{p1}(x, y, \mathbf{r}_{He}(z, t), t) = \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) + \tilde{\mathbf{r}}_{He}^{p1}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t).$$

and

$$\begin{aligned} \mathbf{r}_{He}^{p2}(x, y, z, t) &= \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_{He}^{p2}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t) \\ &= \mathbf{r}_{He}(z, t) + \hat{\mathbf{r}}_{He}^{p2}(x, y, \mathbf{r}_{He}(z, t), t), \end{aligned} \quad (29)$$

where

$$\hat{\mathbf{r}}_{He}^{p2}(x, y, \mathbf{r}_{He}(z, t), t) = \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) + \tilde{\mathbf{r}}_{He}^{p2}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t).$$

For the Helium neutron fields, we denote

$$\begin{aligned} \mathbf{r}_{He}^{N1}(x, y, z, t) &= \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_{He}^{N1}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t) \\ &= \mathbf{r}_{He}(z, t) + \hat{\mathbf{r}}_{He}^{N1}(x, y, \mathbf{r}_{He}(z, t), t), \end{aligned} \quad (30)$$

where

$$\hat{\mathbf{r}}_{He}^{N1}(x, y, \mathbf{r}_{He}(z, t), t) = \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) + \tilde{\mathbf{r}}_{He}^{N1}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t).$$

and

$$\begin{aligned} \mathbf{r}_{He}^{N2}(x, y, z, t) &= \mathbf{r}_{He}(z, t) + \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) \\ &\quad + \tilde{\mathbf{r}}_{He}^{N2}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t) \\ &= \mathbf{r}_{He}(z, t) + \hat{\mathbf{r}}_{He}^{N2}(x, y, \mathbf{r}_{He}(z, t), t), \end{aligned} \quad (31)$$

where

$$\hat{\mathbf{r}}_{He}^{N2}(x, y, \mathbf{r}_{He}(z, t), t) = \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t) + \tilde{\mathbf{r}}_{He}^{N2}(x, \mathbf{r}_{He}^A(y, \mathbf{r}_{He}(z, t), t), \mathbf{r}_{He}(z, t), t).$$

For the neutron field

$$\mathbf{r}_N(y, z, t) = \mathbf{r}_N^M(z, t) + \hat{\mathbf{r}}_N(y, \mathbf{r}_N^M(z, t), t)$$

Finally, for the electronic field resulting from ionization,

$$\mathbf{r}_e(y, z, t) = \mathbf{r}_e^M(z, t) + \hat{\mathbf{r}}_e(y, \mathbf{r}_e^M(z, t), t)$$

The system is subject to the following constraints

$$\int_{\Omega} |\hat{\phi}_D^p(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_D^N(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_T^p(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_T^{N_1}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_T^{N_2}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{H_e}^{p_1}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{H_e}^{p_2}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{H_e}^{N_1}(x, y, z, t)|^2 dx = 1,$$

$$\int_{\Omega} |\hat{\phi}_{H_e}^{N_2}(x, y, z, t)|^2 dx = 1,$$

in $\Omega \times \Omega \times [0, t_f]$,

$$\int_{\Omega} |\hat{\phi}_N(y, z, t)|^2 dy = 1,$$

$$\int_{\Omega} |\hat{\phi}_e(y, z, t)|^2 dy = 1,$$

$$\int_{\Omega} |\phi_D^A(y, z, t)|^2 dy = 1,$$

$$\int_{\Omega} |\phi_T^A(y, z, t)|^2 dy = 1,$$

and

$$\int_{\Omega} |\hat{\phi}_{H_e}^A(y, z, t)|^2 dy = 1,$$

in $\Omega \times [0, t_f]$.

Defining

$$m_D(t) = \int_{\Omega} |\phi_D(z, t)|^2 dz,$$

$$m_T(t) = \int_{\Omega} |\phi_T(z, t)|^2 dz,$$

$$m_{H_e}(t) = \int_{\Omega} |\phi(z, t)_{H_e}|^2 dz,$$

$$m_N(t) = \int_{\Omega} |\phi_N^M(z, t)|^2 dz,$$

and

$$m_e(t) = \int_{\Omega} |\phi_e^M(z, t)|^2 dz,$$

and also defining

$$\rho_D(\mathbf{r}_D(z, t), t) = |\phi_D(z, t)|^2,$$

$$\rho_T(\mathbf{r}_T(z, t), t) = |\phi_T(z, t)|^2,$$

$$\rho_{H_e}(\mathbf{r}_{H_e}(z, t), t) = |\phi_{H_e}(z, t)|^2,$$

$$\rho_N^M(\mathbf{r}_N^M(z, t), t) = |\phi_N^M(z, t)|^2,$$

$$\rho_e^M(\mathbf{r}_e^M(z, t), t) = |\phi_e^M(z, t)|^2,$$

and

$$\mathbf{v}_D(\mathbf{r}_D(z, t), t) = \frac{\partial \mathbf{r}_D(z, t)}{\partial t},$$

$$\mathbf{v}_T(\mathbf{r}_T(z, t), t) = \frac{\partial \mathbf{r}_T(z, t)}{\partial t},$$

$$\mathbf{v}_{H_e}(\mathbf{r}_{H_e}(z, t), t) = \frac{\partial \mathbf{r}_{H_e}(z, t)}{\partial t},$$

$$\mathbf{v}_N(\mathbf{r}_N^M(z, t), t) = \frac{\partial \mathbf{r}_N^M(z, t)}{\partial t},$$

and

$$\mathbf{v}_e(\mathbf{r}_e^M(z, t), t) = \frac{\partial \mathbf{r}_e^M(z, t)}{\partial t},$$

other constraints may be expressed by

$$\begin{aligned} m_D(t) &= (m_0)_D - \int_0^t \int_{\partial\Omega} \rho_D(\mathbf{r}_D(z, \tau), \tau) \mathbf{v}_D(\mathbf{r}_D(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \\ &\quad - \alpha_D [m_{H_e}(t) + m_N(t)] \\ &\quad - \alpha_D \int_0^t \int_{\partial\Omega} \rho_{H_e}(\mathbf{r}_{H_e}(z, \tau), \tau) \mathbf{v}_{H_e}(\mathbf{r}_{H_e}(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \\ &\quad - \alpha_D \int_0^t \int_{\partial\Omega} \rho_N^M(\mathbf{r}_N^M(z, \tau), \tau) \mathbf{v}_N(\mathbf{r}_N^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \end{aligned} \quad (32)$$

$$\begin{aligned}
 m_T(t) = & (m_0)_T - \int_0^t \int_{\partial\Omega} \rho_T(\mathbf{r}_T(z, \tau), \tau) \mathbf{v}_T(\mathbf{r}(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \\
 & - \alpha_T [m_{H_e}(t) + m_N(t)] \\
 & - \alpha_T \int_0^t \int_{\partial\Omega} \rho_{H_e}(\mathbf{r}_{H_e}(z, \tau), \tau) \mathbf{v}_{H_e}(\mathbf{r}_{H_e}(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \\
 & - \alpha_T \int_0^t \int_{\partial\Omega} \rho_N^M(\mathbf{r}_N^M(z, \tau), \tau) \mathbf{v}_N(\mathbf{r}_N^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \quad (33)
 \end{aligned}$$

$$\begin{aligned}
 & \alpha_N \left(m_{H_e}(t) + \int_0^t \int_{\partial\Omega} \rho_{H_e}(\mathbf{r}_{H_e}(z, \tau), \tau) \mathbf{v}_{H_e}(\mathbf{r}_{H_e}(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right) \\
 = & \alpha_{H_e} \left(m_N(t) + \int_0^t \int_{\partial\Omega} \rho_N^M(\mathbf{r}_N^M(z, \tau), \tau) \mathbf{v}_N(\mathbf{r}_N^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right) \quad (34)
 \end{aligned}$$

$$m_e(t) = (m_0)_e - \int_0^t \int_{\partial\Omega} \rho_e^M(\mathbf{r}_e^M(z, \tau), \tau) \mathbf{v}_e(\mathbf{r}_e^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau, \quad (35)$$

where $\mathbf{n}$ denotes the outward normal field to $\partial\Omega = S$.

At this point, we define the kinetics energy functional E_C by

$$\begin{aligned}
 E_C = & \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^p \frac{\partial \mathbf{r}_D^p}{\partial t} \cdot \frac{\partial \mathbf{r}_D^p}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^N \frac{\partial \mathbf{r}_D^N}{\partial t} \cdot \frac{\partial \mathbf{r}_D^N}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^p \frac{\partial \mathbf{r}_T^p}{\partial t} \cdot \frac{\partial \mathbf{r}_T^p}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_1} \frac{\partial \mathbf{r}_T^{N_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_T^{N_1}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_2} \frac{\partial \mathbf{r}_T^{N_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_T^{N_2}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{p_1} \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{p_2} \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_1} \frac{\partial \mathbf{r}_{He}^{N_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{N_1}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_2} \frac{\partial \mathbf{r}_{He}^{N_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}^{N_2}}{\partial t} dx dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_N \frac{\partial \mathbf{r}_N}{\partial t} \cdot \frac{\partial \mathbf{r}_N}{\partial t} dy dz dt \\
 & + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_e \frac{\partial \mathbf{r}_e}{\partial t} \cdot \frac{\partial \mathbf{r}_e}{\partial t} dy dz dt,
 \end{aligned} \tag{36}$$

We may expand such an expression obtaining

$$E_C = E_{C_1} + E_{C_2} + E_{C_3}$$

where

$$\begin{aligned}
E_{C_1} = & \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_D \frac{\partial \mathbf{r}_D}{\partial t} \cdot \frac{\partial \mathbf{r}_D}{\partial t} dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \rho_T \frac{\partial \mathbf{r}_T}{\partial t} \cdot \frac{\partial \mathbf{r}_T}{\partial t} dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \rho_{He} \frac{\partial \mathbf{r}_{He}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}}{\partial t} dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \rho_N \frac{\partial \mathbf{r}_N^M}{\partial t} \cdot \frac{\partial \mathbf{r}_N^M}{\partial t} dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \rho_e \frac{\partial \mathbf{r}_e^M}{\partial t} \cdot \frac{\partial \mathbf{r}_e^M}{\partial t} dz dt,
\end{aligned} \tag{37}$$

$$\begin{aligned}
E_{C_2} = & \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^p \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^N \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^p \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_1} \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_2} \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \hat{\rho}_{He}^{p_1} \frac{\partial \hat{\mathbf{r}}_{He}^{p_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{p_1}}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{p_2} \frac{\partial \hat{\mathbf{r}}_{He}^{p_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{p_2}}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_1} \frac{\partial \hat{\mathbf{r}}_{He}^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{N_1}}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_2} \frac{\partial \hat{\mathbf{r}}_{He}^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{He}^{N_2}}{\partial t} dx dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_N \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_N}{\partial t} dy dz dt \\
& + \frac{1}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_e \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_e}{\partial t} dy dz dt,
\end{aligned} \tag{38}$$

and

$$\begin{aligned}
 E_{C_3} = & \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^p \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \cdot \frac{\partial \mathbf{r}_D}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_D^N \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \cdot \frac{\partial \mathbf{r}_D}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^p \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \cdot \frac{\partial \mathbf{r}_T}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_1} \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_T}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_T^{N_2} \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_T}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{p_1} \frac{\partial \hat{\mathbf{r}}_{He}^{p_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{p_2} \frac{\partial \hat{\mathbf{r}}_{He}^{p_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_1} \frac{\partial \hat{\mathbf{r}}_{He}^{N_1}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} \rho_{He}^{N_2} \frac{\partial \hat{\mathbf{r}}_{He}^{N_2}}{\partial t} \cdot \frac{\partial \mathbf{r}_{He}}{\partial t} dx dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_N \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \cdot \frac{\partial \mathbf{r}_N^M}{\partial t} dy dz dt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} \rho_e \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \cdot \frac{\partial \mathbf{r}_e^M}{\partial t} dy dz dt,
 \end{aligned} \tag{39}$$

Here we define the functional E_q where

$$\begin{aligned}
 E_q = & \frac{\gamma_D^p}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_D^p - iw_D^p \mathbf{A}(z, t) \phi_D^p|^2 dx dy dz dt \\
 & + \frac{\gamma_D^N}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_D^N - iw_D^N \mathbf{A}(z, t) \phi_D^N|^2 dx dy dz dt \\
 & + \frac{\gamma_T^p}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_T^p - iw_T^p \mathbf{A}(z, t) \phi_T^p|^2 dx dy dz dt \\
 & + \frac{\gamma_T^{N_1}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_T^{N_1} - iw_T^{N_1} \mathbf{A}(z, t) \phi_T^{N_1}|^2 dx dy dz dt \\
 & + \frac{\gamma_T^{N_2}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_T^{N_2} - iw_T^{N_2} \mathbf{A}(z, t) \phi_T^{N_2}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{p_1}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{p_1} - iw_{H_e}^{p_1} \mathbf{A}(z, t) \phi_{H_e}^{p_1}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{p_2}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{p_2} - iw_{H_e}^{p_2} \mathbf{A}(z, t) \phi_{H_e}^{p_2}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{N_1}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{N_1} - iw_{H_e}^{N_1} \mathbf{A}(z, t) \phi_{H_e}^{N_1}|^2 dx dy dz dt \\
 & + \frac{\gamma_{H_e}^{N_2}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_x \phi_{H_e}^{N_2} - iw_{H_e}^{N_2} \mathbf{A}(z, t) \phi_{H_e}^{N_2}|^2 dx dy dz dt \\
 & + \frac{\gamma_N}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_N - iw_N \mathbf{A}(z, t) \phi_N|^2 dy dz dt \\
 & + \frac{\gamma_e}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_e - iw_e \phi_e \mathbf{A}(z, t) \phi_e|^2 dy dz dt \\
 & + \frac{\gamma_D^A}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_D^A - iw_D^A \mathbf{A}(z, t) \phi_D^A|^2 dy dz dt \\
 & + \frac{\gamma_T^A}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_T^A - iw_T^A \mathbf{A}(z, t) \phi_T^A|^2 dy dz dt \\
 & + \frac{\gamma_{H_e}^A}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_y \phi_{H_e}^A - iw_{H_e}^A \mathbf{A}(z, t) \phi_{H_e}^A|^2 dy dz dt \\
 & + \frac{\gamma_D}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_D - iw_D \mathbf{A}(z, t) \phi_D|^2 dz dt \\
 & + \frac{\gamma_T}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_T - iw_T \mathbf{A}(z, t) \phi_T|^2 dz dt \\
 & + \frac{\gamma_{H_e}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_{H_e} - iw_{H_e} \mathbf{A}(z, t) \phi_{H_e}|^2 dz dt \\
 & + \frac{\gamma_N^M}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_N^M - iw_N^M \mathbf{A}(z, t) \phi_N^M|^2 dz dt \\
 & + \frac{\gamma_e^M}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\nabla_z \phi_e^M - iw_N^M \mathbf{A}(z, t) \phi_e^M|^2 dz dt.
 \end{aligned} \tag{40}$$

We define also,

$$\begin{aligned}
 E_{q_1} = & \frac{\gamma_D^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_D}{\partial t} \cdot \frac{\partial \phi_D}{\partial t} dz dt \\
 & + \frac{\gamma_T^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_T}{\partial t} \cdot \frac{\partial \phi_T}{\partial t} dz dt \\
 & + \frac{\gamma_{He}^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_{He}}{\partial t} \cdot \frac{\partial \phi_{He}}{\partial t} dz dt \\
 & + \frac{\gamma_N^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_N^M}{\partial t} \cdot \frac{\partial \phi_N^M}{\partial t} dx dt \\
 & + \frac{\gamma_e^0}{2} \int_0^{t_f} \int_{\Omega} \frac{\partial \phi_e^M}{\partial t} \cdot \frac{\partial \phi_e^M}{\partial t} dz dt.
 \end{aligned} \tag{41}$$

For the interaction energy functional we consider only a simplified self interaction part, denoted by E_{int} , where

$$\begin{aligned}
 E_{int} = & \frac{\alpha_D}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_D|^4 dx dy dz dt \\
 & + \frac{\alpha_T}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_T|^4 dx dy dz dt \\
 & + \frac{\alpha_{He}}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}|^4 dx dy dz dt \\
 & + \frac{\alpha_N}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\phi_N|^4 dy dz dt \\
 & + \frac{\alpha_e}{2} \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\phi_e|^4 dy dz dt.
 \end{aligned} \tag{42}$$

Furthermore, concerning the scalar temperature field, we define

$$\begin{aligned}
 (C_v)_D \rho_D(z, t) T_D(z, t) = & \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^p|^2 \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \right) dx dy \\
 & + \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^N|^2 \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \right) dx dy
 \end{aligned} \tag{43}$$

$$\begin{aligned}
 (C_v)_T \rho_T(z, t) T_T(z, t) = & \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^p|^2 \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \right) dx dy \\
 & + \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \right) dx dy \\
 & + \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \right) dx dy
 \end{aligned} \tag{44}$$

$$\begin{aligned}
(C_v)_{H_e} \rho_{H_e}(z, t) T_{H_e}(z, t) &= \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{p_1}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_1}}{\partial t} \right) dx dy \\
&+ \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{p_2}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_2}}{\partial t} \right) dx dy \\
&+ \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_1}}{\partial t} \right) dx dy \\
&+ \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_2}}{\partial t} \right) dx dy \quad (45)
\end{aligned}$$

$$(C_v)_N \rho_N^M(z, t) T_N(z, t) = \int_{\Omega} \left(\frac{1}{2} |\phi_N|^2 \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \right) dy \quad (46)$$

$$(C_v)_e \rho_e^M(z, t) T_e = \int_{\Omega} \left(\frac{1}{2} |\phi_e|^2 \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \right) dy \quad (47)$$

Moreover, we define

$$T(z, t) = T_D + T_T + T_{H_e} + T_N + T_e$$

and similarly as indicated in [16] for a non-viscous fluid, we also assume the following constraint

$$\begin{aligned}
&|\phi_D|^2 (C_v)_D \frac{\partial T_D}{\partial t} + |\phi_T|^2 (C_v)_T \frac{\partial T_T}{\partial t} \\
&+ |\phi_{H_e}|^2 (C_v)_{H_e} \frac{\partial T_{H_e}}{\partial t} + |\phi_N|^2 (C_v)_N \frac{\partial T_N}{\partial t} + |\phi_e|^2 (C_v)_e \frac{\partial T_e}{\partial t} \\
&- K_D \nabla^2 T_D - K_T \nabla^2 T_T - K_{H_e} \nabla^2 T_{H_e} - K_N \nabla^2 T_N - K_e \nabla^2 T_e \\
&+ P_D \operatorname{div} \mathbf{v}_D + P_T \operatorname{div} \mathbf{v}_T + P_{H_e} \operatorname{div} \mathbf{v}_{H_e} \\
&+ P_N \operatorname{div} \mathbf{v}_N + P_e \operatorname{div} \mathbf{v}_e - \frac{\partial Q}{\partial t} = 0, \text{ in } \Omega \times [0, t_f], \quad (48)
\end{aligned}$$

where Q is a heat function and

$$\begin{aligned}
P_D &= \frac{d(\hat{P} \rho_D)}{dt}, \\
P_T &= \frac{d(\hat{P} \rho_T)}{dt}, \\
P_{H_e} &= \frac{d(\hat{P} \rho_{H_e})}{dt},
\end{aligned}$$

$$P_N = \frac{d(\hat{P}\rho_N)}{dt},$$

and

$$P_e = \frac{d(\hat{P}\rho_e)}{dt}.$$

Finally, we assume the following mass conservation equation as a constraint

$$\begin{aligned} & \frac{d\rho}{dt} + \rho_D \operatorname{div}(\mathbf{v}_D) + \rho_T \operatorname{div}(\mathbf{v}_T) \\ & + \rho_{H_e} \operatorname{div}(\mathbf{v}_{H_e}) + \rho_N \operatorname{div}(\mathbf{v}_N) \\ & + \rho_e \operatorname{div}(\mathbf{v}_e) = 0, \text{ in } \Omega \times [0, t_f], \end{aligned} \quad (49)$$

where we recall to have denoted

$$\rho = \rho_D + \rho_T + \rho_{H_e} + \rho_N + \rho_e$$

and

$$\begin{aligned} \rho_D &= \rho_D(\mathbf{r}_D(z, t), t), \\ \rho_T &= \rho_T(\mathbf{r}_T(z, t), t), \\ \rho_{H_e} &= \rho_{H_e}(\mathbf{r}_{H_e}(z, t), t), \\ \rho_N &= \rho_N(\mathbf{r}_N^M(z, t), t), \end{aligned}$$

and

$$\rho_e = \rho_e(\mathbf{r}_e^M(z, t), t).$$

In order to model such a chemical reaction, we define the following functional J , which corresponds to a variational formulation for the model in question, where

$$\begin{aligned}
J = & E_{C_1} + E_{C_2} + E_{C_3} + E_q + E_{q_1} + E_{int} \\
& - \int_0^{t_f} \int_{\Omega} \hat{P} \left(\frac{d\rho}{dt} + \rho_D \operatorname{div}(\mathbf{v}_D) + \rho_T \operatorname{div}(\mathbf{v}_T) \right. \\
& + \rho_{H_e} \operatorname{div}(\mathbf{v}_{H_e}) + \rho_N \operatorname{div}(\mathbf{v}_N) \\
& \left. + \rho_e \operatorname{div}(\mathbf{v}_e) \right) dzdt \\
& - \int_0^{t_f} \int_{\Omega} \mathbf{g} \cdot (\rho_D \mathbf{r}_D + \rho_T \mathbf{r}_T + \rho_{H_e} \mathbf{r}_{H_e} + \rho_N \mathbf{r}_N^M + \rho_e \mathbf{r}_e^M) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_1 \left(\mathbf{v}_D(\mathbf{r}_D(z, t), t) - \frac{\partial \mathbf{r}_D(z, t)}{\partial t} \right) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_2 \left(\mathbf{v}_T(\mathbf{r}_T(z, t), t) - \frac{\partial \mathbf{r}_T(z, t)}{\partial t} \right) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_3 \left(\mathbf{v}_{H_e}(\mathbf{r}_{H_e}(z, t), t) - \frac{\partial \mathbf{r}_{H_e}(z, t)}{\partial t} \right) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_4 \left(\mathbf{v}_N(\mathbf{r}_N^M(z, t), t) - \frac{\partial \mathbf{r}_N^M(z, t)}{\partial t} \right) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_5 \left(\mathbf{v}_e(\mathbf{r}_e^M(z, t), t) - \frac{\partial \mathbf{r}_e^M(z, t)}{\partial t} \right) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_6 (\rho_D(\mathbf{r}_D(z, t), t) - |\phi_D(z, t)|^2) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_7 (\rho_T(\mathbf{r}_T(z, t), t) - |\phi_T(z, t)|^2) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_8 (\rho_{H_e}(\mathbf{r}_{H_e}(z, t), t) - |\phi_{H_e}(z, t)|^2) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_9 (\rho_N(\mathbf{r}_N^M(z, t), t) - |\phi_N^M(z, t)|^2) dzdt \\
& + \int_0^{t_f} \int_{\Omega} \hat{\lambda}_{10} (\rho_e(\mathbf{r}_e^M(z, t), t) - |\phi_e^M(z, t)|^2) dzdt \\
& + J_{Aux_1} + J_{Aux_2} + J_{Aux_3} + J_{Aux_4} + J_{Aux_5} + J_{Aux_6}, \tag{50}
\end{aligned}$$

where

$$\begin{aligned}
& J_{Aux_1} \\
= & \int_0^{t_f} \int_{\Omega} \lambda_D \left((C_v)_D \rho_D(z, t) T_D(z, t) - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^p|^2 \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^p}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_D^N|^2 \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_D^N}{\partial t} \right) dx dy \right) dz dt \\
& - \int_0^{t_f} \int_{\Omega} \lambda_T \left((C_v)_T \rho_T(z, t) T_T(z, t) - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^p|^2 \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^p}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_1}}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_T^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_T^{N_2}}{\partial t} \right) dx dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_{H_e} \left((C_v)_{H_e} \rho_{H_e}(z, t) T_{H_e}(z, t) - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{p_1}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_1}}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{p_2}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{p_2}}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{N_1}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_1}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_1}}{\partial t} \right) dx dy \right. \\
& \left. - \int_{\Omega} \int_{\Omega} \left(\frac{1}{2} |\phi_{H_e}^{N_2}|^2 \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_2}}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_{H_e}^{N_2}}{\partial t} \right) dx dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_N \left((C_v)_N \rho_N^M(z, t) T_N(z, t) - \int_{\Omega} \left(\frac{1}{2} |\phi_N|^2 \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_N}{\partial t} \right) dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_e \left((C_v)_e \rho_e^M(z, t) T_e - \int_{\Omega} \left(\frac{1}{2} |\phi_e|^2 \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \cdot \frac{\partial \hat{\mathbf{r}}_e}{\partial t} \right) dy \right) dz dt \\
& + \int_0^{t_f} \int_{\Omega} \lambda_1 \left(|\phi_D|^2 (C_v)_D \frac{\partial T_D}{\partial t} + |\phi_T|^2 (C_v)_T \frac{\partial T_T}{\partial t} \right. \\
& + |\phi_{H_e}|^2 (C_v)_{H_e} \frac{\partial T_{H_e}}{\partial t} + |\phi_N|^2 (C_v)_N \frac{\partial T_N}{\partial t} + |\phi_e|^2 (C_v)_e \frac{\partial T_e}{\partial t} \\
& - K_D \nabla^2 T_D - K_T \nabla^2 T_T - K_{H_e} \nabla^2 T_{H_e} - K_N \nabla^2 T_N - K_e \nabla^2 T_e \\
& + P_D \operatorname{div} \mathbf{v}_D + P_T \operatorname{div} \mathbf{v}_T + P_{H_e} \operatorname{div} \mathbf{v}_{H_e} \\
& \left. + P_N \operatorname{div} \mathbf{v}_N + P_e \operatorname{div} \mathbf{v}_e - \frac{\partial Q}{\partial t} \right) dz dt, \tag{51}
\end{aligned}$$

Moreover,

$$\begin{aligned}
 & J_{Aux_2} \\
 = & \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_D^p(y, z, t) \left(\int_{\Omega} |\hat{\phi}_D^p(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_D^p(y, z, t) \left(\int_{\Omega} |\hat{\phi}_D^N(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_T^p(y, z, t) \left(\int_{\Omega} |\hat{\phi}_T^p(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_T^{N_1}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_T^{N_1}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_T^{N_2}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_T^{N_2}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{p_1}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{p_1}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{p_2}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{p_2}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{N_1}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{N_1}(x, y, z, t)|^2 dx - 1 \right) dydzdt \\
 & + \int_0^{t_f} \int_{\Omega} \int_{\Omega} E_{H_e}^{N_2}(y, z, t) \left(\int_{\Omega} |\hat{\phi}_{H_e}^{N_2}(x, y, z, t)|^2 dx - 1 \right) dydzdt \quad (52)
 \end{aligned}$$

$$\begin{aligned}
 & J_{Aux_3} \\
 = & \int_0^{t_f} \int_{\Omega} E_N(z, t) \left(\int_{\Omega} \int_{\Omega} |\hat{\phi}_N(y, z, t)|^2 dy - 1 \right) dzdt, \\
 & + \int_0^{t_f} \int_{\Omega} E_e(z, t) \left(\int_{\Omega} |\hat{\phi}_e(y, , z, t)|^2 dy - 1 \right) dzdt, \\
 & + \int_0^{t_f} \int_{\Omega} E_D^A(z, t) \left(\int_{\Omega} |\phi_D^A(y, z, t)|^2 dy - 1 \right) dzdt \\
 & + \int_0^{t_f} \int_{\Omega} E_T^A(z, t) \left(\int_{\Omega} |\phi_T^A(y, z, t)|^2 dy - 1 \right) dzdt \\
 & + \int_0^{t_f} \int_{\Omega} E_{H_e}^A(z, t) \left(\int_{\Omega} |\phi_{H_e}^A(y, z, t)|^2 dy - 1 \right) dzdt \quad (53)
 \end{aligned}$$

and denoting

$$\begin{aligned}
J_{Aux_4} = & \int_0^{t_f} \mu_D(t) \left(m_D(t) - (m_0)_D + \int_0^t \int_{\partial\Omega} \rho_D(\mathbf{r}_D(z, \tau), \tau) \mathbf{v}_D(\mathbf{r}_D(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right. \\
& + \alpha_D [m_{He}(t) + m_N(t)] - \alpha_D \int_0^t \int_{\partial\Omega} \rho_{He}(\mathbf{r}_{He}(z, \tau), \tau) \mathbf{v}_{He}(\mathbf{r}_{He}(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \\
& \left. + \alpha_D \int_0^t \int_{\partial\Omega} \rho_N(\mathbf{r}_N^M(z, \tau), \tau) \mathbf{v}_N(\mathbf{r}_N^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right) dt \\
& + \int_0^{t_f} \mu_T(t) \left(m_T(t) - (m_0)_T + \int_0^t \int_{\partial\Omega} \rho_T(\mathbf{r}_T(z, \tau), \tau) \mathbf{v}_T(\mathbf{r}_T(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right. \\
& + \alpha_T [m_{He}(t) + m_N(t)] + \alpha_T \int_0^t \int_{\partial\Omega} \rho_{He}(\mathbf{r}_{He}(z, \tau), \tau) \mathbf{v}_{He}(z, \tau) \cdot \mathbf{n} dS d\tau \\
& \left. + \alpha_T \int_0^t \int_{\partial\Omega} \rho_N(\mathbf{r}_N^M(z, \tau), \tau) \mathbf{v}_N(\mathbf{r}_N^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right) dt \\
& + \int_0^{t_f} \mu_3(t) \left(\alpha_N \left(m_{He}(t) + \int_0^t \int_{\partial\Omega} \rho_{He}(\mathbf{r}_{He}(z, \tau), \tau) \mathbf{v}_{He}(\mathbf{r}_{He}(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right) \right. \\
& \left. - \alpha_{He} \left(m_N(t) + \int_0^t \int_{\partial\Omega} \rho_N(\mathbf{r}_N^M(z, \tau), \tau) \mathbf{v}_N(\mathbf{r}_N^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right) \right) dt \\
& + \int_0^{t_f} \mu_4(t) (m_e(t) - (m_0)_e \\
& \left. + \int_0^t \int_{\partial\Omega} \rho_e^M(\mathbf{r}_e^M(z, \tau), \tau) \mathbf{v}_e(\mathbf{r}_e^M(z, \tau), \tau) \cdot \mathbf{n} dS d\tau \right) dt. \tag{54}
\end{aligned}$$

Furthermore,

$$\begin{aligned}
 & J_{Aux5} \\
 = & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} V(\mathbf{r}_D^p, \mathbf{r}_T^p, \mathbf{r}_{He}^{p_1}, \mathbf{r}_{He}^{p_2}, \mathbf{r}_e) \\
 & \times (|\phi_D^p|^2 + |\phi_T^p|^2 + |\phi_{He}^{p_1}|^2 + |\phi_{He}^{p_2}|^2 + |\phi_e|^2) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_D^p|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_D^p}{\partial t} \cdot (\mathbf{r}_D^p(z, \varepsilon t) - (\mathbf{r}_0)_D^p) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_T^p|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_T^p}{\partial t} \cdot (\mathbf{r}_T^p(z, \varepsilon t) - (\mathbf{r}_0)_T^p) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_1}|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} \cdot (\mathbf{r}_{He}^{p_1}(z, \varepsilon t) - (\mathbf{r}_0)_{He}^{p_1}) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_2}|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} \cdot (\mathbf{r}_{He}^{p_2}(z, \varepsilon t) - (\mathbf{r}_0)_{He}^{p_2}) dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_e|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_e}{\partial t} \cdot (\mathbf{r}_e(z, \varepsilon t) - (\mathbf{r}_0)_e) dx dy dz dt \\
 & + \frac{1}{8\pi} \int_0^{t_f} \int_{\Omega} |\text{curl } \mathbf{A}(z, t) - \mathbf{B}_0(z, t)|^2 dz dt \\
 & + \frac{1}{8\pi} \int_0^{t_f} \int_{\Omega} \left| \int_{\Omega} \int_{\Omega} \nabla_z V(\mathbf{r}_D^p, \mathbf{r}_T^p, \mathbf{r}_{He}^{p_1}, \mathbf{r}_{He}^{p_2}, \mathbf{r}_e) dx dy + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right|^2 dz dt, \quad (55)
 \end{aligned}$$

where

$$\mathbf{B}(z, t) = \text{curl } \mathbf{A}(z, t) - \mathbf{B}_0(z, t)$$

is the total magnetic field,

$$\mathbf{A} = (A_1, A_2, A_3) \in W^{1,2}(\Omega \times [0, t_f]; \mathbb{R}^3)$$

denotes the magnetic potential and

$$\mathbf{E} = - \int_{\Omega} \int_{\Omega} \nabla_z V(\mathbf{r}_D^p, \mathbf{r}_T^p, \mathbf{r}_{He}^{p_1}, \mathbf{r}_{He}^{p_2}, \mathbf{r}_e) dx dy - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t},$$

denotes the electric field.

Finally,

$$\begin{aligned}
 J_{Aux_6} = & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_D^p|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_D^p}{\partial t} dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_T^p|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_T^p}{\partial t} dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_1}|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_{He}^{p_1}}{\partial t} dx dy dz dt \\
 & -K_1 \int_0^{t_f} \int_{\Omega} \int_{\Omega} \int_{\Omega} |\phi_{He}^{p_2}|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_{He}^{p_2}}{\partial t} dx dy dz dt \\
 & -K_2 \int_0^{t_f} \int_{\Omega} \int_{\Omega} |\phi_e|^2 \mathbf{A} \cdot \frac{\partial \mathbf{r}_e}{\partial t} dy dz dt. \tag{56}
 \end{aligned}$$

Remark 3.1. About the domain of the functional J , we generically define it as sets of smooth C^2 functions, specifying only the following boundary and initial conditions

$$\mathbf{r} = (\mathbf{r}_D, \mathbf{r}_T, \mathbf{r}_{He}, \mathbf{r}_N^M, \mathbf{r}_e^M) = \mathbf{0}, \text{ on } \partial\Omega \times [0, t_f],$$

$$\mathbf{r}|_{t=0} = z, \text{ in } \Omega,$$

$$\mathbf{v} = (\mathbf{v}_D, \mathbf{v}_T, \mathbf{v}_{He}, \mathbf{v}_N^M, \mathbf{v}_e^M) = \mathbf{0}, \text{ on } \partial\Omega_1 \times [0, t_f],$$

where

$$S = \partial\Omega = \partial\Omega_1 \cup \partial\Omega_2,$$

$$\mathbf{v}|_{t=0} = \mathbf{v}_0 \text{ in } \Omega,$$

$$T = T_0(z, t) \text{ on } \partial\Omega \times [0, t_f]$$

$$T|_{t=0} = T_1(z), \text{ in } \Omega$$

and

$$\rho|_{t=0} = (\rho_D, \rho_T, \rho_{He}, \rho_N, \rho_e)|_{t=0} = ((\rho_D)_0, (\rho_T)_0, 0, 0, (\rho_e)_0) \text{ in } \Omega.$$

Remark 3.2. Concerning the variation of J in $\mathbf{r}$, we consider variations in the context

$$(\mathbf{r} + h\varphi) \text{ and } (\mathbf{r}(\cdot, \varepsilon t) + h\varphi),$$

that is, the same variable variation φ and real constant h for both $\mathbf{r}$ and $\mathbf{r}(\cdot, \varepsilon t)$ for obtaining an approximate Euler-Lagrange equation. Finally, letting $\varepsilon \rightarrow 0$ we obtain the correct Euler-Lagrange equation.

3.1 About some of the Euler-Lagrange equations

The variation of J in $\mathbf{v}_D$ stands for

$$\rho_D \mathbf{v}_D + \hat{\lambda}_1 + \nabla(\rho_D \hat{P}) - \nabla(\lambda_1 P_D) = \mathbf{0},$$

in $\Omega \times [0, t_f]$.

Symbolically, the variation of J in $\mathbf{r}_D$ stands for

$$\begin{aligned} \frac{dJ}{d\mathbf{r}_D} &= \frac{\partial J}{\partial \mathbf{v}} \frac{\partial \mathbf{v}}{\partial \mathbf{r}_D} + \frac{\partial J}{\partial \rho} \frac{\partial \rho}{\partial \mathbf{r}_D} + \frac{\partial J}{\partial \mathbf{r}_D} \\ &= \frac{\partial J}{\partial \mathbf{r}_D} \\ &= \mathbf{0}, \end{aligned} \tag{57}$$

that is,

$$\begin{aligned} & \frac{\partial \hat{\lambda}_1}{\partial t} - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^p \frac{d\hat{\mathbf{r}}_D^p}{dt} \right) dx dy \\ & - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^N \frac{d\hat{\mathbf{r}}_D^N}{dt} \right) dx dy \\ & - K_1 \int_{\Omega} \int_{\Omega} \left(|\phi_D|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_D^p}{\partial t} \right) dx dy \\ & - \int_{\Omega} \int_{\Omega} \left(K_1 \frac{\partial V}{\partial \mathbf{r}_D} (|\phi_D^p|^2 + |\phi_T^p|^2 + |\phi_{He}^{p1}|^2 + |\phi_{He}^{p2}|^2 + |\phi_e|^2) \right. \\ & \quad \left. + \frac{1}{4\pi} \operatorname{div}(\mathbf{E}) \frac{\partial V}{\partial \mathbf{r}_D} \right) dx dy \\ & + K_1 \frac{\partial}{\partial t} (|\phi_D|^2 \mathbf{A}) + \mathcal{O}(\varepsilon) - \rho_D \mathbf{g} \\ & = \mathbf{0} \end{aligned} \tag{58}$$

Letting $\varepsilon \rightarrow 0$ and considering a Maxwell equation in question, we obtain

$$\begin{aligned} & \frac{\partial \hat{\lambda}_1}{\partial t} - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^p \frac{d\hat{\mathbf{r}}_D^p}{dt} \right) dx dy \\ & - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^N \frac{d\hat{\mathbf{r}}_D^N}{dt} \right) dx dy - K_1 \int_{\Omega} \int_{\Omega} \left(|\phi_D|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_D^p}{\partial t} \right) dx dy \\ & + K_1 \frac{\partial}{\partial t} (|\phi_D|^2 \mathbf{A}) - \rho_D \mathbf{g} = \mathbf{0}, \text{ in } \Omega \times [0, t_f]. \end{aligned} \tag{59}$$

Combining these two last Euler-Lagrange equations we obtain

$$\begin{aligned}
& -\frac{d(\rho_D \mathbf{v}_D)}{dt} - \frac{d(\nabla(\rho_D \hat{P}))}{dt} + \frac{d(\nabla(\lambda_1 P_D))}{dt} \\
& - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^p \frac{d\hat{\mathbf{r}}_D^p}{dt} \right) dx dy \\
& - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^N \frac{d\hat{\mathbf{r}}_D^N}{dt} \right) dx dy - K_1 \int_{\Omega} \int_{\Omega} \left(|\phi_D|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_D^p}{\partial t} \right) dx dy \\
& + K_1 \frac{\partial}{\partial t} (|\phi_D|^2 \mathbf{A}) - \rho_D \mathbf{g} = \mathbf{0}, \text{ in } \Omega \times [0, t_f].
\end{aligned} \tag{60}$$

Thus,

$$\begin{aligned}
& -\frac{\partial(\rho_D \mathbf{v}_D)}{\partial t} - \frac{\partial(\rho_D \mathbf{v}_D)}{\partial(X_D)_k} (v_D)_k \\
& - \frac{d(\nabla(\rho_D \hat{P}))}{dt} + \frac{d(\nabla(\lambda_1 P_D))}{dt} \\
& - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^p \frac{d(\hat{\mathbf{r}}_D^p)}{dt} \right) dx dy \\
& - \int_{\Omega} \int_{\Omega} \frac{d}{dt} \left(\rho_D^N \frac{d(\hat{\mathbf{r}}_D^N)}{dt} \right) dx dy \\
& - K_1 \int_{\Omega} \int_{\Omega} \left(|\phi_D|^2 \mathbf{B} \times \frac{\partial \mathbf{r}_D^p}{\partial t} \right) dx dy \\
& + K_1 \frac{\partial}{\partial t} (|\phi_D|^2 \mathbf{A}) - \rho_D \mathbf{g} = \mathbf{0}, \text{ in } \Omega \times [0, t_f].
\end{aligned} \tag{61}$$

From such a result, considering an Eulerian identification

$$\mathbf{r}_D(z, t) = (X_D(z, t), Y_D(z, t), Z_D(z, t)) \approx z,$$

we finally obtain the Eulerian equation

$$\begin{aligned}
& -\frac{\partial(\rho_D \mathbf{v}_D)}{\partial t} - \frac{\partial(\rho_D \mathbf{v}_D)}{\partial z_k} (v_D)_k \\
& -\nabla P_D + \frac{d(\nabla(\lambda_1 P_D))}{dt} \\
& - \int_{\Omega} \int_{\Omega} \left(\frac{\partial(\rho_D^p \hat{\mathbf{v}}_D^p)}{\partial t} + \frac{\partial(\rho_D^p \hat{\mathbf{v}}_D^p)}{\partial z_k} (v_D)_k \right) dx dy \\
& - \int_{\Omega} \int_{\Omega} \left(\frac{\partial(\rho_D^N \hat{\mathbf{v}}_D^N)}{\partial t} + \frac{\partial(\rho_D^N \hat{\mathbf{v}}_D^N)}{\partial z_k} (v_D)_k \right) dx dy \\
& - K_1 \int_{\Omega} \int_{\Omega} (|\phi_D|^2 \mathbf{B} \times \mathbf{v}_D^p) dx dy \\
& + K_1 \frac{\partial}{\partial t} (|\phi_D|^2 \mathbf{A}) - \rho_D \mathbf{g} = \mathbf{0}, \text{ in } \Omega \times [0, t_f].
\end{aligned} \tag{62}$$

Moreover, from the variation of J in ρ_D , we obtain

$$\frac{\mathbf{v}_D \cdot \mathbf{v}_D}{2} + \frac{d\hat{P}}{dt} - \hat{P} \operatorname{div} (\mathbf{v}_D) - \mathbf{g} \cdot \mathbf{r}_D + \lambda_6 = 0, \tag{63}$$

in $\Omega \times [0, t_f]$.

Here we recall that

$$P_D = \frac{d(\hat{P} \rho_D)}{dt}.$$

Therefore

$$P_D = \frac{d\hat{P}}{dt} \rho_D + \hat{P} \frac{d\rho_D}{dt},$$

so that

$$\frac{d\hat{P}}{dt} = \frac{P_D}{\rho_D} - \frac{\hat{P}}{\rho_D} \frac{d\rho_D}{dt}.$$

From this and the last Euler-Lagrange equation, we have

$$\frac{\mathbf{v}_D \cdot \mathbf{v}_D}{2} + \frac{P_D}{\rho_D} - \frac{\hat{P}}{\rho_D} \frac{d\rho_D}{dt} - \hat{P} \operatorname{div} (\mathbf{v}_D) + g Z_D(z, t) + \lambda_6 = 0, \tag{64}$$

in $\Omega \times [0, t_f]$.

From such a result and the previously indicated Eulerian identification we finally obtain

$$\frac{\mathbf{v}_D \cdot \mathbf{v}_D}{2} + \frac{P_D}{\rho_D} - \frac{\hat{P}}{\rho_D} \left(\frac{d\rho_D}{dt} + \rho_D \operatorname{div} (\mathbf{v}_D) \right) + g z + \lambda_6 = 0, \tag{65}$$

in $\Omega \times [0, t_f]$.

This last equation is a kind of a generalization of the Bernoulli one concerning the present context.

Similar results may be obtained for the remaining Euler-Lagrange equations for J .

4 Conclusion

In this article we have developed variational formulations for modeling a hydrogen nuclear fusion through a high temperature process. In the last sections, our approach here presented has been non-relativistic and in an Eulerian context.

In a near future research we intend to develop similar results in a relativistic context.

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